How Grain Growth Stops: A New Solution to an Old Mystery

Controlling grain size is a fundamental problem in materials science with technological implications.

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Most metals and ceramics are polycrystalline; they are comprised of many individual crystallites, called grains. The sizes, shapes and arrangement of these grains are important to the properties of the material – sometimes more important than the chemical composition. Understanding and controlling grain structure is important to nearly every engineered material. For materials that rely on strength, such as structural steel, a very fine grain size is desirable. On the other hand, there are important systems, such as silicon photovoltaics (Figure 1), in which a large, or even single crystal, grain size is preferred. Because the grain structure governs how a material performs, materials scientists have studied how to manipulate it for nearly two centuries. However, there are limits to how far the grain structure can be modified. For example, it is very difficult to create extremely small or large grains. While the lower limit of grain size is well understood – it is set by the atomic scale – the upper limit of grain size remains a mystery. Why can't grains grow beyond a certain size?

Grains are separated by interfaces called grain boundaries. Because atomic bonds are broken at grain boundaries, they contribute energy to the system. That implies that the lowest energy state of the system should contain no grain boundaries; in other words, the equilibrium state of most metals and ceramics should be a single crystal. When polycrystalline materials are heated to sufficiently high temperatures, the grain boundaries move and rearrange so as to decrease the amount of grain boundary present. However, even at very high temperatures and very long times, grain growth rarely proceeds to the single crystal state. Instead, grain growth nearly always stops even though many grains remain. Why grain growth stops is one of the oldest, most fundamental questions in materials science. It's not a purely academic question, either. It is challenging and expensive to make single crystals and usually depends on careful melt processing. If one could create single crystal silicon photocells by a solid-state process, the cost of solar panels would drastically decrease.

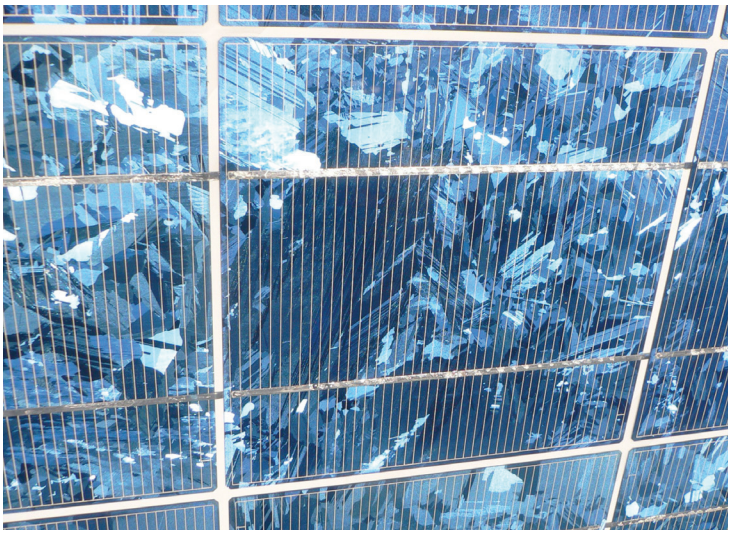

Figure 1: Stagnant grain structures in high-purity silicon photocells; single crystal photocells would be more efficient, but cannot be made by grain growth processing due to grain stagnation.

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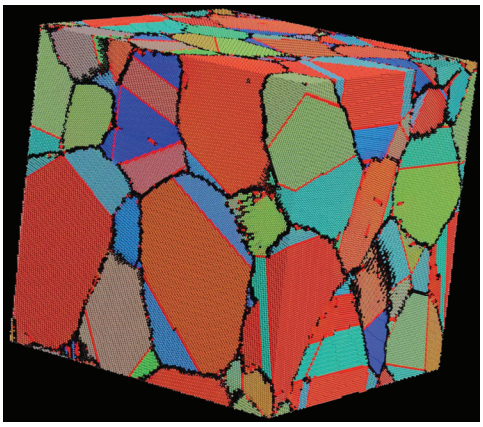

Figure 2: A stagnating grain structure in pure nickel, simulated on the atomic scale. Individual atoms are colored according to their grain membership, with black atoms denoting grain boundaries. Even though grain growth has slowed dramatically, many grains remain, and the structure is far from the equilibrium single crystal state. Previous grain growth models cannot explain the stagnation phenomenon.

There have been many mechanisms proposed for grain growth stagnation, each valid for certain materials and processes. However, none of these mechanisms has been able to explain grain growth stagnation for an important class of materials that includes photovoltaics: polycrystalline materials of very high purity.

At Sandia, a new mechanism has recently been discovered for grain growth stagnation that has not been described, or even speculated upon, before (Reference 1). This insight was enabled by the combination of atomistic and grain-scale simulation and illustrates the power of computational modeling to reveal physical phenomena unattainable by other methods. In recent large-scale simulations of several hundred individual grain boundaries, it was discovered that grain boundaries can be separated into two classes – fast and slow moving– depending on their atomic structure (References 2,3). The proportion of fast and slow boundaries depends on the temperature of the system. A grain-scale simulation was used to determine how the fast/slow ratio changes grain growth when many grains are present. It was found that when all boundaries are fast, growth proceeds to the equilibrium single crystal state. In contrast, if any slow boundaries are present, grain growth stops short of the single crystal, with the fraction of slow boundaries determining how many grains remain – even when the material is perfectly pure.

Because pure materials are hard to come by in the real world, confirmation of the discovery was obtained by using atomistic simulation techniques to build a pure polycrystal from the atoms up. A grain structure was thus constructed containing several hundred interconnected grains and heated to various temperatures. Figure 2 shows the result: Grain size grows at early times, but then slows short of the single crystal state, with the final structure containing many individual grains. The size of the remaining grains is in good agreement with the predictions of grain-scale simulations, as shown in Figure 3. Although this is not conclusive proof that slow boundaries stop grain growth, it is highly suggestive – and no other stagnation mechanism is known in perfectly pure polycrystals.

Because controlling grain size to optimize properties is a fundamental problem in materials science, understanding how grain growth stops is a centuries-old problem. While a number of mechanisms have been proposed, slow grain boundary stagnation is the first new stagnation mechanism proposed in half a century and the only one to explain how grain growth stops in perfectly pure materials. With this new insight, materials scientists can begin to understand – and hopefully control – grain growth stagnation in important classes of engineered materials.

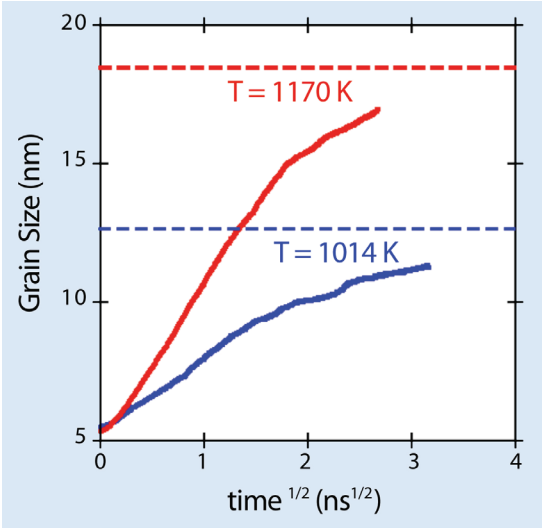

Figure 3: In atomic-scale simulations at two different temperatures, grain size increases for a while and then slows dramatically at later times, as shown by the solid lines. The grain size at stagnation agrees well with the predictions of a grain-scale model based on slow boundaries, shown as dashed lines. This agreement suggests that slow boundaries can stop grain growth even in perfectly pure materials.

References

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